SEARCH REQUEST FORM

Access DB# 54957

Scientific and Technical Information Center

RECEIVED NOV 15 2001 TC/CREN (STIC)

Requester's Full Name: Jeffrey E. Russel Examiner #: 62785 Date: 11-15-2001

Art Unit: 1653 Phone Number 308-3975 Serial Number: 09/623506

Mail Box and Bldg/Room Location: CM1-7801/CM1-7807 Results Format Preferred (circle): PAPER-DISK-E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

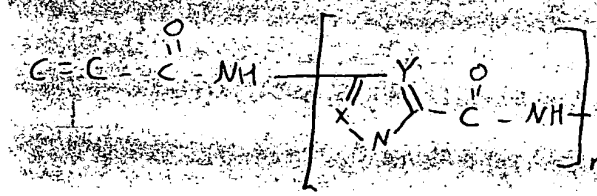
Title of Invention: Acrylol Derivatives Analogous To Distamycin, And Their Use As Antitumor Agents

Inventors (please provide full names): F. Gozzi; P. Barali; I. Berta; M. Calderelli; L. Cepeloni; R. Ronzoni

Earliest Priority Filing Date: 9-19-2000

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Please search the following partial structure:



where X = N and Y = CH, or X = CH and Y = N.

Please search for n = 1. If there are too many hits please narrow by requiring n = 2.

Keywords are cancer, antitumor, tumor, antineoplastic, carcinoma

Thank you.

****

STAFF USE ONLY

Searcher: Shaporia

Searcher Phone #: 308-4499

Searcher Location:

Date Searcher Picked Up:

Date Completed: 11/16/01

Searcher Prep & Review Time:

Clerical Prep Time:

Online Time:

Type of Search

NA Sequence (#)

AA Sequence (#)

Structure (#)

Bibliographic

Litigation

Fulltext

Patent Family

Other

Vendors and cost where applicable

STN

Dialog

Questel/Orbit

Dr.Link

Lexis/Nexis

Sequence Systems

WWW/Internet

Other (specify)

PTO-1590 (8-01)

=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 16:42:07 ON 16 NOV 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1947 - 16 Nov 2001 VOL 135 ISS 22
FILE LAST UPDATED: 15 Nov 2001 (20011115/ED)

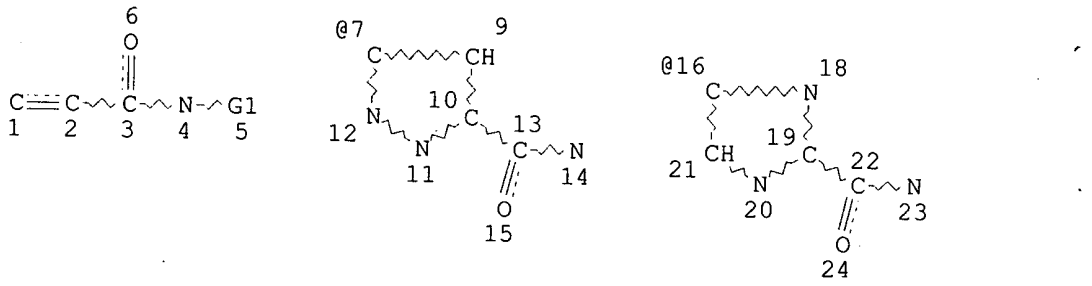
This file contains CAS Registry Numbers for easy and accurate substance identification.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

HCAplus now provides online access to patents and literature covered in CA from 1947 to the present. On April 22, 2001, bibliographic information and abstracts were added for over 2.2 million references published in CA from 1947 to 1966.

=>
=>

=> d stat que l5
L1 STR



VAR G1=7/16
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE
L3 97 SEA FILE=REGISTRY SSS FUL L1
L4 9 SEA FILE=HCAPLUS ABB=ON PLU=ON L3
L5 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L4 AND (?CANCER? OR ?TUMOR? OR ?TUMOUR? OR ?NEOPLAS? OR ?MALIG?)

=>
=>

=> d ibib abs hitrn 15 1-5

L5 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2000:425860 HCAPLUS
DOCUMENT NUMBER: 133:232356
TITLE: Synthesis and **Antitumor** Activity of New Benzoheterocyclic Derivatives of Distamycin A
AUTHOR(S): Baraldi, Pier Giovanni; Romagnoli, Romeo; Beria, Italo; Cozzi, Paolo; Geroni, Cristina; Mongelli, Nicola; Bianchi, Nicoletta; Mischiati, Carlo; Gambari, Roberto
CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche and Dipartimento di Biochimica e Biologia Molecolare, Universita di Ferrara, Ferrara, 44100, Italy
SOURCE: J. Med. Chem. (2000), 43(14), 2675-2684
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:232356

AB The design, synthesis, and in vivo and in vitro antileukemic activity of a novel series of compds. in which different benzoheterocyclic rings, bearing a nitrogen mustard or a benzoyl nitrogen mustard or an .alpha.-bromoacryloyl group as alkylating moieties, are tethered to a distamycin frame are reported, and structure-activity relationships are discussed. The new derivs. were prepd. by coupling nitrogen mustard-substituted, benzoyl nitrogen mustard-substituted, or .alpha.-bromoacryloyl-substituted benzoheterocyclic carboxylic acids with desformyldistamycin or in one case with its two-pyrrole analog. With very few exceptions, the activities of compds. bearing the same alkylating moiety are slightly affected by the kind of the heteroatom present on the benzoheterocyclic ring. All novel compds., with one exception, showed in vitro activity against L1210 murine leukemia cell line comparable to or better than that of tallimustine. The compds. in which the nitrogen mustard and the .alpha.-bromoacryloyl moieties are directly linked to benzoheterocyclic ring showed potent cytotoxic activities (IC50 ranging from 2 to 14 nM), while benzoyl nitrogen mustard derivs. of benzoheterocycles showed reduced cytotoxic activities, and one compd. of this cluster was the sole deriv. devoid of significant activity. A 5-nitrogen mustard N-methylindole deriv. of distamycin, showed the best antileukemic activity in vivo, with a very long survival time (%T/C = 457), significantly increased in comparison to tallimustine (%T/C = 133), and was selected for further extensive evaluation. Arrested polymerase chain reaction and direct DNA fragmentation assays were performed for the 5-nitrogen mustard N-methylindole deriv. of distamycin and structurally related compds. The results obtained have shown that both alkylating groups and oligopeptide frames play a crucial role in the sequence selectivity of these compds.

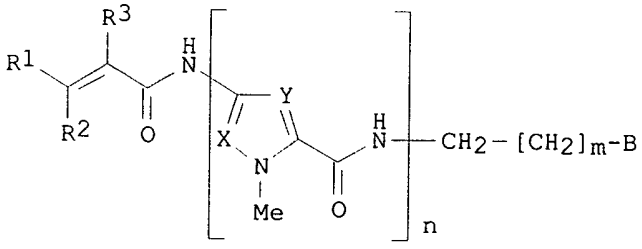
IT **177409-55-1 177409-56-2**
RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(synthesis and **antitumor** activity of new benzoheterocyclic derivs. of distamycin A in relation to structure and DNA sequence selectivity of alkylating groups)

REFERENCE COUNT: 34
REFERENCE(S):
(2) Arcamone, F; Gazz Chim Ital 1967, V97, P1097 HCAPLUS
(3) Arcamone, F; J Med Chem 1989, V32, P774 HCAPLUS
(5) Baraldi, P; Biorg Med Chem Lett 1996, V6, P1241 HCAPLUS
(6) Baraldi, P; Curr Pharm Des 1998, V4, P249 HCAPLUS
(7) Bianchi, N; J Steriod Biochem Mol Biol 1995, V54, P211 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1999:640855 HCAPLUS
DOCUMENT NUMBER: 131:257879
TITLE: Preparation of distamycin acryloyl derivatives as **antitumor** agents
INVENTOR(S): Cozzi, Paolo; Baraldi, Pier Giovanni; Beria, Italo; Caldarelli, Marina; Capolongo, Laura; Romagnoli, Romeo
PATENT ASSIGNEE(S): Pharmacia & Upjohn S.p.A., Italy
SOURCE: PCT Int. Appl., 64 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9950265	A1	19991007	WO 1999-EP1822	19990317
W: AE, AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9934154	A1	19991018	AU 1999-34154	19990317
EP 1064280	A1	20010103	EP 1999-915664	19990317
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				

PRIORITY APPLN. INFO.: GB 1998-6689 A 19980327
WO 1999-EP1822 W 19990317
OTHER SOURCE(S): MARPAT 131:257879
GI



I

AB Distamycin acryloyl derivs. I [n = 2-4; m = 1 or 2; X, Y = N or CH,

selected independently for each heterocyclic ring; R1, R2 = H, halo, alkyl; R3 = H, halo; B = C(NH2):NCN, C(NR4R5):NR6, C(NH2):NNH2, CONR7R8, NHC(NH2):NR9, NR10R11, C(NH2):NOR12, CN; R4-8 and R10-12 are H or alkyl and R9 is H or OH] or their pharmaceutically acceptable salts were prepd. as **antitumor** agents. Thus, treatment of cyanamide with NaH in DMF, followed by addn. of distamycin A and hydrolysis of the formyl group with aq. HCl afforded an amino deriv., which was treated with 1-methyl-3-(.alpha.-bromoacrylamido)pyrrole-5-carbonyl chloride (prepn. given) to give I [n = 4, m = 1, X = Y = CH, R1 = R2 = H, R3 = Br, B = C(NH2):NCN].

IT **177409-55-1**
RL: RCT (Reactant)
(prepn. of distamycin acryloyl derivs. as **antitumor** agents)

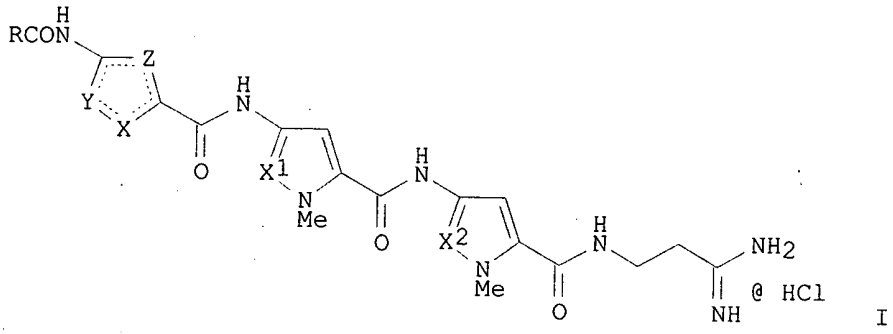
IT **245046-46-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of distamycin acryloyl derivs. as **antitumor** agents)

IT **245045-54-9P 245045-55-0P 245045-56-1P**
245045-58-3P 245045-59-4P 245045-60-7P
245045-61-8P 245045-62-9P 245045-63-0P
245045-64-1P 245045-65-2P 245045-66-3P
245045-67-4P 245045-68-5P 245045-69-6P
245045-70-9P 245045-71-0P 245045-72-1P
245045-73-2P 245045-74-3P 245045-76-5P
245045-77-6P 245045-78-7P 245045-79-8P
245045-80-1P 245045-81-2P 245045-82-3P
245045-83-4P 245045-84-5P 245045-85-6P
245045-86-7P 245045-87-8P 245045-88-9P
245045-89-0P 245045-90-3P 245045-91-4P
245045-93-6P 245045-94-7P 245045-95-8P
245045-96-9P 245045-97-0P 245045-98-1P
245045-99-2P 245046-00-8P 245046-01-9P
245046-10-0P 245046-12-2P 245046-13-3P
245046-14-4P 245046-15-5P 245046-16-6P
245046-17-7P 245046-18-8P 245046-19-9P
245046-20-2P 245046-21-3P 245046-22-4P
245046-23-5P 245046-24-6P 245046-25-7P
245046-26-8P 245046-27-9P 245046-28-0P
245046-29-1P 245046-30-4P 245046-31-5P
245046-32-6P 245046-34-8P 245046-35-9P
245046-36-0P 245046-37-1P 245046-38-2P
245046-42-8P 245046-44-0P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of distamycin acryloyl derivs. as **antitumor** agents)

REFERENCE COUNT: 4
REFERENCE(S):
(1) Marina, C; WO 9804524 A 1998 HCAPLUS
(2) Pharmacia Spa; WO 9605196 A 1996 HCAPLUS
(3) Pharmacia & Upjohn Spa; WO 9743258 A 1997 HCAPLUS
(4) Synphar Lab Inc; WO 9504732 A 1995 HCAPLUS

L5 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1996:368758 HCAPLUS
DOCUMENT NUMBER: 125:143281
TITLE: Structure-activity relationship of novel tallimustine derivatives: synthesis and **antitumor** activity
AUTHOR(S): Baraldi, Pier Giovanni; Beria, Italo; Cacciari, Barbara; Coplongo, Laura; Cozzi, Paolo; Nogelli, Nicola; Romagnoli, Romeo; Spalluto, Giampiero

CORPORATE SOURCE: Dip. Sci. Farm., Univ. Ferrara, Ferrara, 44100, Italy
SOURCE: Bioorg. Med. Chem. Lett. (1996), 6(11), 1247-1252
CODEN: BMCLE8; ISSN: 0960-894X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

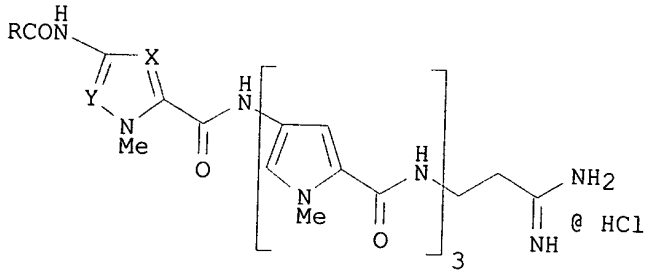


I

AB Oligopeptide-like derivs. I [R = 4-(ClCH2CH2)2NC6H4, CH2:CBr; X = NMe, X = X1 = X2 = N, Y = Z = CH; X = X1 = CH, X2 = N, CH, Y = S, Z = N; X = NMe, X1 = Y = Z = CH, X2 = N, CH], structurally related to the **antitumor** agent tallimustine, where one or two pyrrole rings were replaced by pyrazole or thiazole rings and bearing benzoyl nitrogen mustard or bromoacryloyl moieties were synthesized and evaluated in vitro and in vivo against L1210 murine leukemia. Compds. I [R = 4-(ClCH2CH2)2NC6H4; X = NMe; X1 = N, CH; Y = Z = CH; X2 = N] showed **antitumor** activity higher than or comparable with that of tallimustine.

IT **177409-54-0P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and **antitumor** structure-activity relationships of tallimustine azole derivs.)

L5 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1996:368757 HCAPLUS
DOCUMENT NUMBER: 125:143280
TITLE: Synthesis and **antitumor** activity of novel distamycin derivatives
AUTHOR(S): Baraldi, Pier Giovanni; Beria, Italo; Cacciari, Barbara; Cozzi, Paolo; Franzetti, Cristina; Mongelli, Nicola; Romagnoli, Romeo; Spalluto, Giampiero
CORPORATE SOURCE: Dip. Sci. Farm., Univ. Ferrara, Ferrara, 44100, Italy
SOURCE: Bioorg. Med. Chem. Lett. (1996), 6(11), 1241-1246
CODEN: BMCLE8; ISSN: 0960-894X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Several distamycin derivs. I [Y = N, X = CH; Y = CH, X = N; R = 4-(ClCH2CH2)2NC6H4, CH2:CBr] were synthesized from deformyldistamycin by coupling with different azolecarboxylic acids bearing an alkylating moiety. Some of them showed good activities in vitro and in vivo against L 1210 murine leukemia.

IT **177409-55-1P 177409-56-2P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and **antitumor** activity of novel distamycin derivs.)

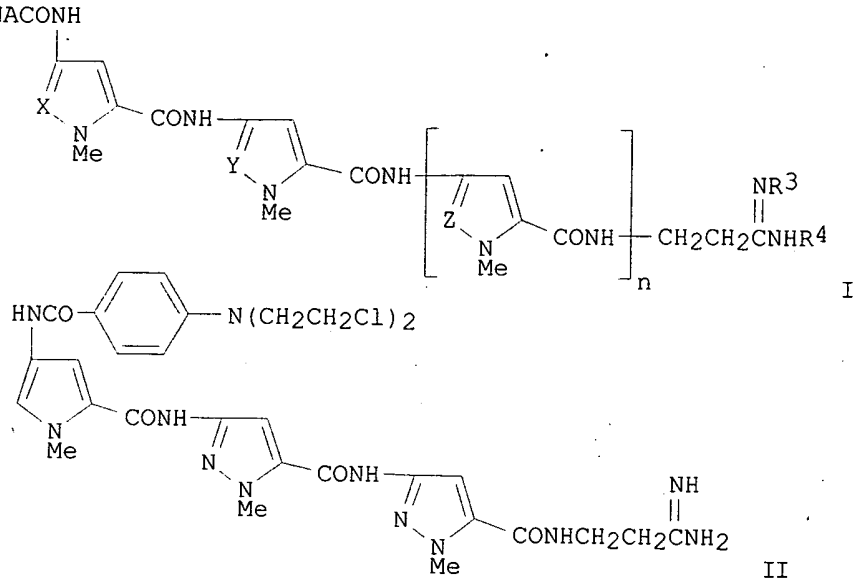
L5 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1996:342035 HCAPLUS
DOCUMENT NUMBER: 125:10484
TITLE: Distamycin A analogs as **antitumor** or antiviral agents
INVENTOR(S): Beria, Italo; Pesenti, Enrico; Capolongo, Laura; Mongelli, Nicola; Baraldi, Piergiovanni
PATENT ASSIGNEE(S): Pharmacia S.P.A., Italy
SOURCE: PCT Int. Appl., 96 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9605196	A1	19960222	WO 1995-EP2814	19950718
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SI, SK, TJ, TT, UA, US, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2172629	AA	19960222	CA 1995-2172629	19950718
AU 9531136	A1	19960307	AU 1995-31136	19950718
AU 689623	B2	19980402		
EP 722446	A1	19960724	EP 1995-926927	19950718
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, NL, PT, SE				
CN 1131946	A	19960925	CN 1995-190742	19950718
JP 09504039	T2	19970422	JP 1995-506945	19950718
HU 76267	A2	19970728	HU 1996-1218	19950718
ZA 9506590	A	19960318	ZA 1995-6590	19950807
US 5753629	A	19980519	US 1996-612836	19960318
NO 9601377	A	19960530	NO 1996-1377	19960403
FI 9601506	A	19960605	FI 1996-1506	19960403

PRIORITY APPLN. INFO.: GB 1994-16005 19940808
WO 1995-EP2814 19950718

OTHER SOURCE(S): MARPAT 125:10484

GI



AB Title compds. I [n = 0, 1; X, Y, Z = N, CH; A = (un)substituted 5-membered heterocycle; R1, R2 = alkyl, haloalkyl, hydroxyalkyl, H, aziridinylalkylcarbonyl, cyclopropylalkylcarbonyl, alkenyl, haloalkenyl, (un)substituted oxiranyl, (un)substituted aminophenyl; R3, R4 = H; R3R4 = CH2CH2, (CH2)3, CH:CH] and their pharmaceutically acceptable salt were prepd. Thus, the pyrrole deriv. II was obtained by treating the nitropyrrolecarboxylic acid fragment with the pyrazolecarboxamidopyrazolecarboxamidopropionitrile, converting the nitrile to the amidine, reducing the nitro group, and acylating. II had an ID50 against L1210 murine leukemia in vitro of 0.5 .mu.g/mL.

IT **177409-54-0P 177409-55-1P 177409-56-2P**
177409-77-7P 177409-82-4P 177409-83-5P
177409-84-6P 177409-86-8P 177409-87-9P
177409-88-0P 177409-99-3P 177410-01-4P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of distamycin analogs as **neoplasm** inhibitors)

=>
=>

=> select hit rn 15 1-5
E5 THROUGH E91 ASSIGNED

=>
=>

=> d ibib abs hitrn l6 1-4

L6 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2001:327062 HCAPLUS
DOCUMENT NUMBER: 135:102536
TITLE: Sequence-specific DNA interstrand cross-linking by imidazole-pyrrole CPI conjugate
AUTHOR(S): Bando, Toshikazu; Iida, Hirokazu; Saito, Isao; Sugiyama, Hiroshi
CORPORATE SOURCE: CREST Japan Science and Technology Corporation (JST) Japan Division of Biofunctional Molecules Institute of Biomaterials and Bioengineering Tokyo Medical and Dental University, Kanda Chiyoda Tokyo, 101-0062, Japan
SOURCE: J. Am. Chem. Soc. (2001), 123(21), 5158-5159
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB DNA interstrand crosslinking inhibits both DNA replication and gene expression and therefore has considerable potential for mol. biol. and human medicine. However, an interstrand crosslinking agent that targets a predetd. base-pair sequence has not been achieved. Minor-groove binding polyamides that contain N-methylimidazole (Im)-N-methylpyrrole (Py)hydroxypyrrole (Hp), which uniquely recognize each of the four Watson-Crick base pairs, can be used as novel recognition parts of sequence-specific DNA alkylating agents. We also demonstrated that Im/Py diamide-CPI conjugate with a vinyl linker, ImPyLDu86, alkylates double-stranded DNA at predetd. sequences through highly cooperative homodimer formation. Herein we describe the synthesis of a covalent dimer of ImPyLDu86 connected with various linkers and their DNA interstrand crosslinking abilities. In conclusion, we developed a novel DNA interstrand crosslinking agent, that crosslinked double strands only in the presence of ImImPy at a nine-base-pair sequence, 5'-PyGGC(T/A)GCCPu-3'. The present system will provide a promising approach for the design of novel sequence-specific DNA interstrand crosslinking agents. Targeting specific sequences in the human genome by such sequence-specific crosslinking agent would constitute a powerful gene-regulating tool. Further studies on the applicability of this novel class of crosslinking agents are currently in progress.
IT **349647-79-6**
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(sequence-specific DNA interstrand crosslinking by imidazole-pyrrole CPI conjugate)
REFERENCE COUNT: 28
REFERENCE(S):
(1) Boger, D; Angew Chem, Int Ed Engl 1996, V35, P1438 HCAPLUS
(2) Boger, D; Bioorg Med Chem 1995, V3, P1429 HCAPLUS
(3) Boger, D; J Am Chem Soc 1997, V119, P311 HCAPLUS
(4) Boger, D; J Org Chem 1990, V55, P4499 HCAPLUS
(5) Chang, A; J Am Chem Soc 2000, V122, P4856 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2001:28188 HCAPLUS
DOCUMENT NUMBER: 134:207755
TITLE: A General Solution- and Solid-Phase Synthetic

Procedure for Incorporating Three Contiguous Imidazole Moieties into DNA Sequence Reading Polyamides
AUTHOR(S): Sharma, Sanjay K.; Tandon, Manju; Lown, J. William
CORPORATE SOURCE: Department of Chemistry, University of Alberta, Edmonton, AB, T6G 2G2, Can.
SOURCE: J. Org. Chem. (2001), 66(3), 1030-1034
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The authors report a general protocol for the synthesis of imidazole polyamides which could recognize extended GC sequences of DNA with very high affinity. They have linked the three imidazole units by both flexible and rigid linkers. Cellular uptake of products was improved (no data) by adding a natural amidinium end group, introduced by a modified Pinner reaction. To overcome problems of product soly. found with increasing imidazole content, a solid-phase method was developed for a triimidazole-polyamide precursor, resulting in a combined soln./solid-phase method.
IT **329039-02-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of DNA sequence reading polyamides contg. three contiguous imidazole moieties via soln. or solid-phase chem.)
IT **329038-97-3P 329039-05-6P**
RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of DNA sequence reading polyamides contg. three contiguous imidazole moieties via soln. or solid-phase chem.)
REFERENCE COUNT: 48
REFERENCE(S):
(1) Al-Said, N; Synthetic Commun 1995, V25, P1059 HCAPLUS
(2) Al-Said, N; Tetrahedron Lett 1994, V35, P7577 HCAPLUS
(3) Arcamone, F; Gazz Chim Ital 1967, V97, P1097 HCAPLUS
(4) Baird, E; J Am Chem Soc 1996, V118, P6141 HCAPLUS
(5) Chen, Y; J Am Chem Soc 1994, V116, P6995 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 2000:398441 HCAPLUS
DOCUMENT NUMBER: 133:177479
TITLE: Synthesis of geometrically constrained unsymmetrical bis(polyamides) related to the antiviral distamycin
AUTHOR(S): Sharma, Sanjay K.; Tandon, Manju; Lown, J. William
CORPORATE SOURCE: Department of Chemistry, University of Alberta, Edmonton, AB, T6G 2G2, Can.
SOURCE: Eur. J. Org. Chem. (2000), (11), 2095-2103
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:177479
AB Anal. of the structural and stereochem. requirements for the strict DNA base-sequence recognition of (AT)4 and (AT)5, resp., for the oligopeptide minor-groove binding agents netropsin and distamycin leads to proposals for the rational structure modification for altered base recognition. In this paper we report the synthesis of unsym. imidazo-pyrrolo-bis(polyamides), structurally related to the natural antiviral agents distamycin, and bearing either unnatural (25-27) or natural (31-33)

termini linked by a flexible or rigid linker. This is the first report of the synthesis of an imidazole-bearing structure with either (dimethylamino)propyl or amidinium termini in the linked bis(polyamides).

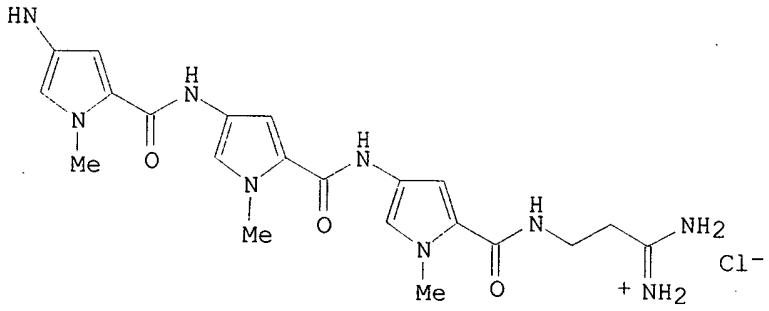
IT **288623-85-8P 288623-92-7P 288624-03-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of geometrically constrained unsym. bis(polyamides) related to distamycin)

IT **288623-99-4P 288624-06-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of geometrically constrained unsym. bis(polyamides) related to distamycin)

REFERENCE COUNT: 24
REFERENCE(S):
(1) Al-Said, N; Synth Commun 1995, V25, P1059 HCAPLUS
(2) Arcamone, F; Gazz Chim Ital 1967, V97, P1097 HCAPLUS
(4) Bryson, T; J Org Chem 1974, V39, P1158 HCAPLUS
(6) Gmeiner, W; J Biomol Struct Dyn 1999, V17, P507 HCAPLUS
(7) Hass, H; J Am Chem Soc 1949, V71, P1767 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1992:512029 HCAPLUS
DOCUMENT NUMBER: 117:112029
TITLE: Anti-HIV-I activity of linked lexitropsins
AUTHOR(S): Wang, Wuyi; Lown, J. William
CORPORATE SOURCE: Dep. Chem., Univ. Alberta, Edmonton, AB, T6G 2G2, Can.
SOURCE: J. Med. Chem. (1992), 35(15), 2890-7
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

R=



AB Five groups of lexitropsin oligopeptides, e.g. RCO(CH2)nCOR (n = 2, 6, 8, 22), have been synthesized that are structurally related to the natural antiviral agents netropsin and distamycin and bearing two such moieties joined by flexible or rigid linkers. Inhibitory activity of these types of agents against murine leukemia retrovirus (MuLV) led to an evaluation of their inhibition of HIV-I in cell culture. The antiretroviral activity of the five different classes of lexitropsins is discussed in terms of their structural differences.

IT **142482-49-3P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and antiviral activity of, against murine leukemia retrovirus)

=>
=>

=> fil caold
FILE 'CAOLD' ENTERED AT 16:44:35 ON 16 NOV 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2001 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGlstRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=>
=>

=> s l3
L7 0 L3

=>
=>
=> fil reg
FILE 'REGISTRY' ENTERED AT 16:45:25 ON 16 NOV 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2001 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 14 NOV 2001 HIGHEST RN 370064-54-3
DICTIONARY FILE UPDATES: 14 NOV 2001 HIGHEST RN 370064-54-3

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d reg l3 tot
1 RN 349647-79-6 REGISTRY
2 RN 329039-05-6 REGISTRY
3 RN 329039-02-3 REGISTRY

4	RN	329038-97-3	REGISTRY
5	RN	288624-06-6	REGISTRY
6	RN	288624-03-3	REGISTRY
7	RN	288623-99-4	REGISTRY
8	RN	288623-92-7	REGISTRY
9	RN	288623-85-8	REGISTRY
10	RN	245046-46-2	REGISTRY
11	RN	245046-44-0	REGISTRY
12	RN	245046-42-8	REGISTRY
13	RN	245046-38-2	REGISTRY
14	RN	245046-37-1	REGISTRY
15	RN	245046-36-0	REGISTRY
16	RN	245046-35-9	REGISTRY
17	RN	245046-34-8	REGISTRY
18	RN	245046-32-6	REGISTRY
19	RN	245046-31-5	REGISTRY
20	RN	245046-30-4	REGISTRY
21	RN	245046-29-1	REGISTRY
22	RN	245046-28-0	REGISTRY
23	RN	245046-27-9	REGISTRY
24	RN	245046-26-8	REGISTRY
25	RN	245046-25-7	REGISTRY
26	RN	245046-24-6	REGISTRY
27	RN	245046-23-5	REGISTRY
28	RN	245046-22-4	REGISTRY
29	RN	245046-21-3	REGISTRY
30	RN	245046-20-2	REGISTRY
31	RN	245046-19-9	REGISTRY
32	RN	245046-18-8	REGISTRY
33	RN	245046-17-7	REGISTRY
34	RN	245046-16-6	REGISTRY
35	RN	245046-15-5	REGISTRY
36	RN	245046-14-4	REGISTRY
37	RN	245046-13-3	REGISTRY
38	RN	245046-12-2	REGISTRY
39	RN	245046-10-0	REGISTRY
40	RN	245046-01-9	REGISTRY
41	RN	245046-00-8	REGISTRY
42	RN	245045-99-2	REGISTRY
43	RN	245045-98-1	REGISTRY
44	RN	245045-97-0	REGISTRY
45	RN	245045-96-9	REGISTRY
46	RN	245045-95-8	REGISTRY
47	RN	245045-94-7	REGISTRY
48	RN	245045-93-6	REGISTRY
49	RN	245045-91-4	REGISTRY
50	RN	245045-90-3	REGISTRY
51	RN	245045-89-0	REGISTRY
52	RN	245045-88-9	REGISTRY
53	RN	245045-87-8	REGISTRY
54	RN	245045-86-7	REGISTRY
55	RN	245045-85-6	REGISTRY
56	RN	245045-84-5	REGISTRY
57	RN	245045-83-4	REGISTRY
58	RN	245045-82-3	REGISTRY
59	RN	245045-81-2	REGISTRY
60	RN	245045-80-1	REGISTRY
61	RN	245045-79-8	REGISTRY
62	RN	245045-78-7	REGISTRY

63	RN	245045-77-6	REGISTRY
64	RN	245045-76-5	REGISTRY
65	RN	245045-74-3	REGISTRY
66	RN	245045-73-2	REGISTRY
67	RN	245045-72-1	REGISTRY
68	RN	245045-71-0	REGISTRY
69	RN	245045-70-9	REGISTRY
70	RN	245045-69-6	REGISTRY
71	RN	245045-68-5	REGISTRY
72	RN	245045-67-4	REGISTRY
73	RN	245045-66-3	REGISTRY
74	RN	245045-65-2	REGISTRY
75	RN	245045-64-1	REGISTRY
76	RN	245045-63-0	REGISTRY
77	RN	245045-62-9	REGISTRY
78	RN	245045-61-8	REGISTRY
79	RN	245045-60-7	REGISTRY
80	RN	245045-59-4	REGISTRY
81	RN	245045-58-3	REGISTRY
82	RN	245045-56-1	REGISTRY
83	RN	245045-55-0	REGISTRY
84	RN	245045-54-9	REGISTRY
85	RN	177410-01-4	REGISTRY
86	RN	177409-99-3	REGISTRY
87	RN	177409-88-0	REGISTRY
88	RN	177409-87-9	REGISTRY
89	RN	177409-86-8	REGISTRY
90	RN	177409-84-6	REGISTRY
91	RN	177409-83-5	REGISTRY
92	RN	177409-82-4	REGISTRY
93	RN	177409-77-7	REGISTRY
94	RN	177409-56-2	REGISTRY
95	RN	177409-55-1	REGISTRY
96	RN	177409-54-0	REGISTRY
97	RN	142482-49-3	REGISTRY

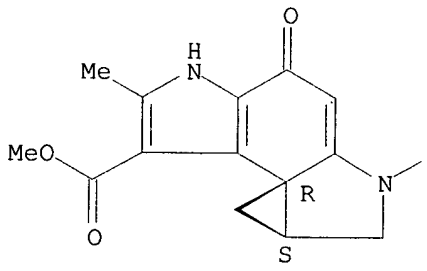
=>
=>

=> d ide can l3 1 2 4 5 7 10 15 20 25 30 35 40 42 45 50 55 60 65 70 75 80 85 86 90 95 97

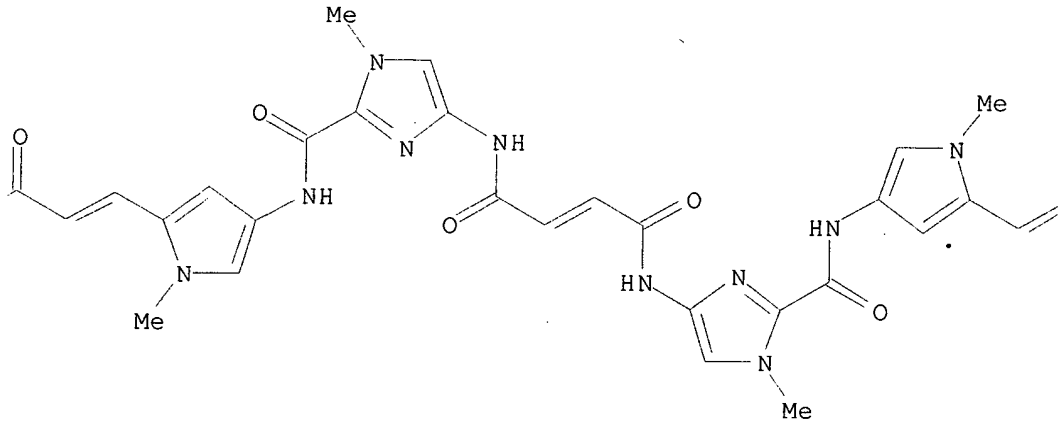
L3 ANSWER 1 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 349647-79-6 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[(1,4-dioxo-2-butene-1,4-diyl)bis[imino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl)(1-oxo-2-propene-3,1-diyl)]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C58 H54 N14 O12
SR CA
LC STN Files: CA, CAPLUS, TOXLIT

Absolute stereochemistry.
Double bond geometry unknown.

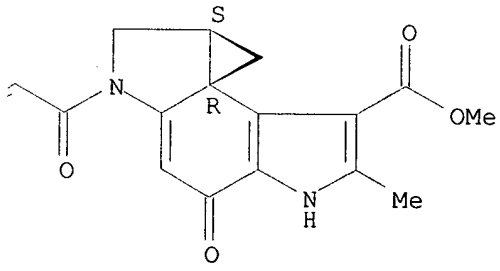
PAGE 1-A



PAGE 1-B



PAGE 1-C



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

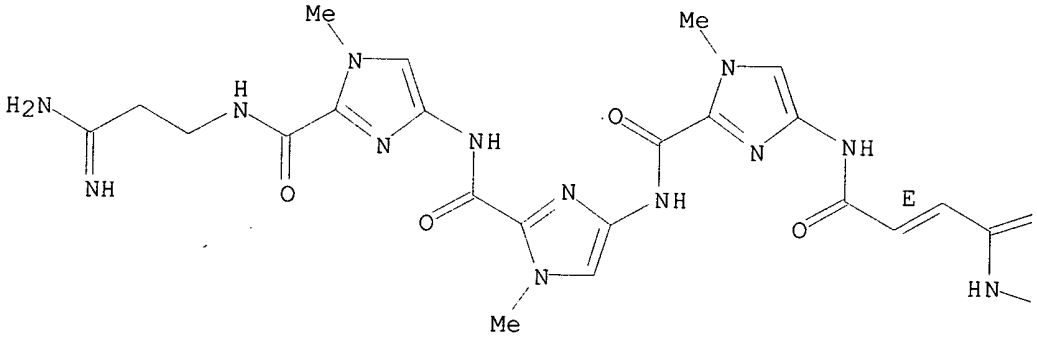
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:102536

L3 ANSWER 2 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 329039-05-6 REGISTRY
CN 2-Butenediamide, N,N'-bis[2-[[[2-[[[2-[[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-imidazol-4-yl]amino]carbonyl]-1-methyl-1H-imidazol-4-yl]amino]carbonyl]-1-methyl-1H-imidazol-4-yl]-, dihydrochloride, (2E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C40 H48 N24 O8 . 2 Cl H
SR CA
LC STN Files: CA, CAPLUS

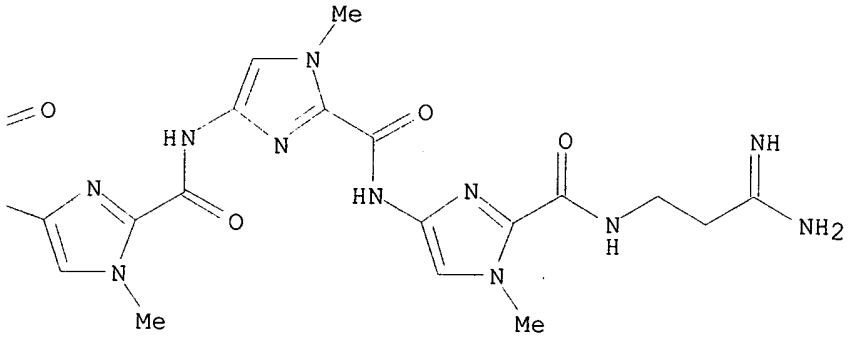
Double bond geometry as shown.

PAGE 1-A



●2 HCl

PAGE 1-B



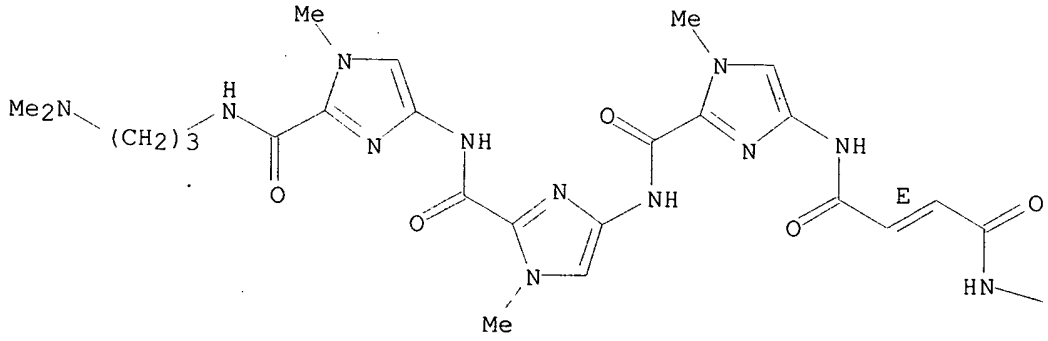
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:207755

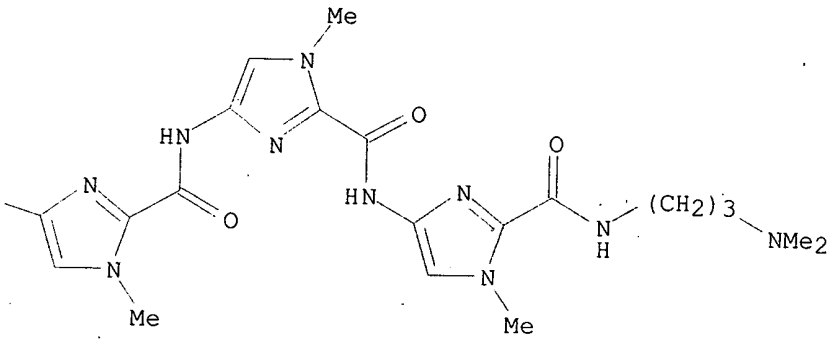
L3 ANSWER 4 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 329038-97-3 REGISTRY
CN 2-Butenediamide, N,N'-bis[2-[[[2-[[[2-[[[3-(dimethylamino)propyl]amino]carbonyl]-1-methyl-1H-imidazol-4-yl]amino]carbonyl]-1-methyl-1H-imidazol-4-yl]amino]carbonyl]-1-methyl-1H-imidazol-4-yl]-, (2E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C44 H58 N22 O8
SR CA
LC STN Files: CA, CAPLUS

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

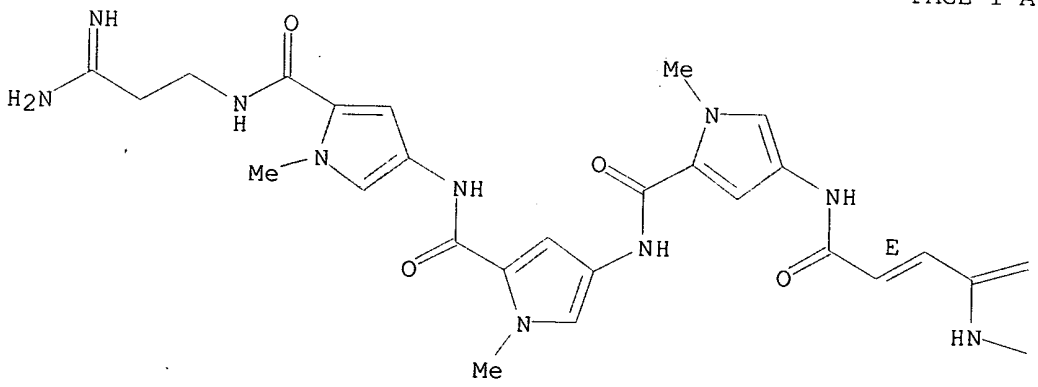
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:207755

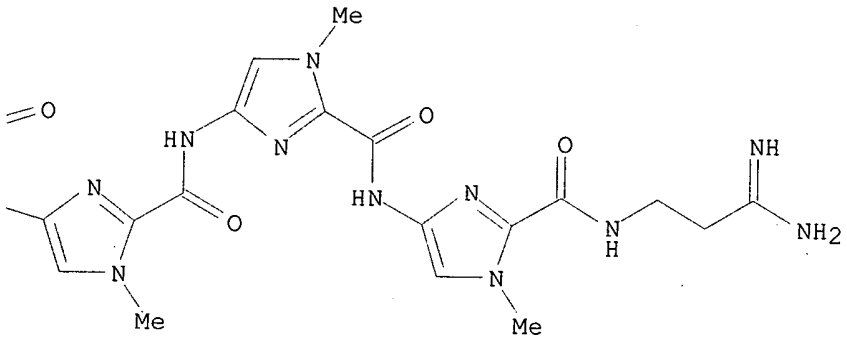
L3 ANSWER 5 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 288624-06-6 REGISTRY
CN 2-Butenediamide, N-[2-[[[2-[[[2-[[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-imidazol-4-yl]amino]carbonyl]-1-methyl-1H-imidazol-4-yl]amino]carbonyl]-1-methyl-1H-imidazol-4-yl]-N'-[5-[[[5-[[[5-[[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-, (2E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C43 H51 N21 O8
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



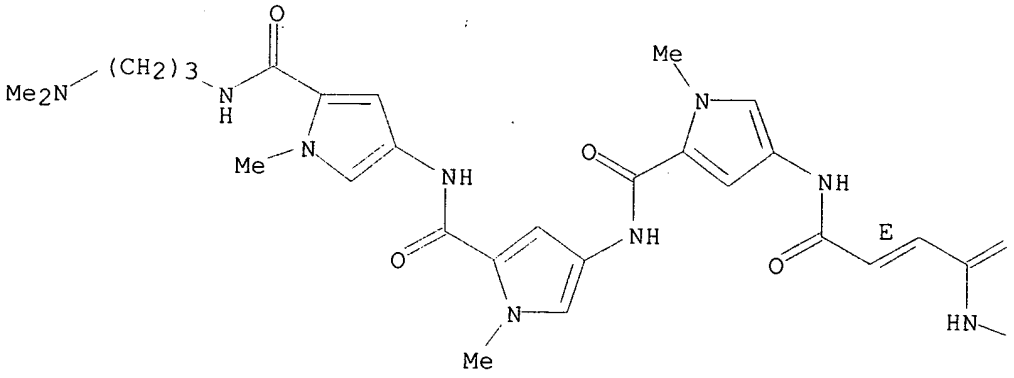
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:177479

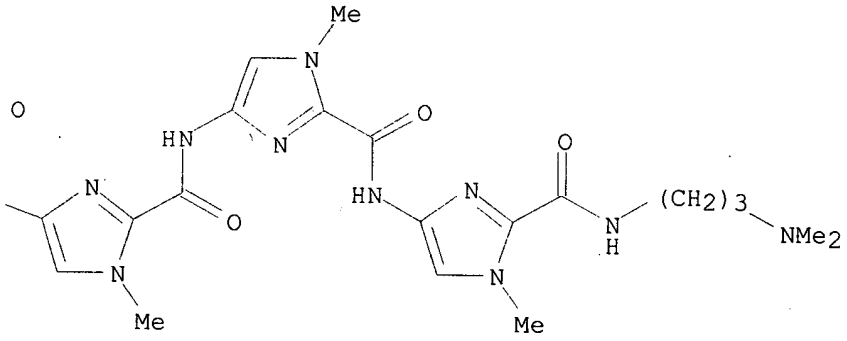
L3 ANSWER 7 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 288623-99-4 REGISTRY
CN 2-Butenediamide, N-[2-[[[2-[[[2-[[[3-(dimethylamino)propyl]amino]carbonyl]-1-methyl-1H-imidazol-4-yl]amino]carbonyl]-1-methyl-1H-imidazol-4-yl]amino]carbonyl]-1-methyl-1H-imidazol-4-yl]-N'-[5-[[[5-[[[5-[[[3-(dimethylamino)propyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-, (2E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C47 H61 N19 O8
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

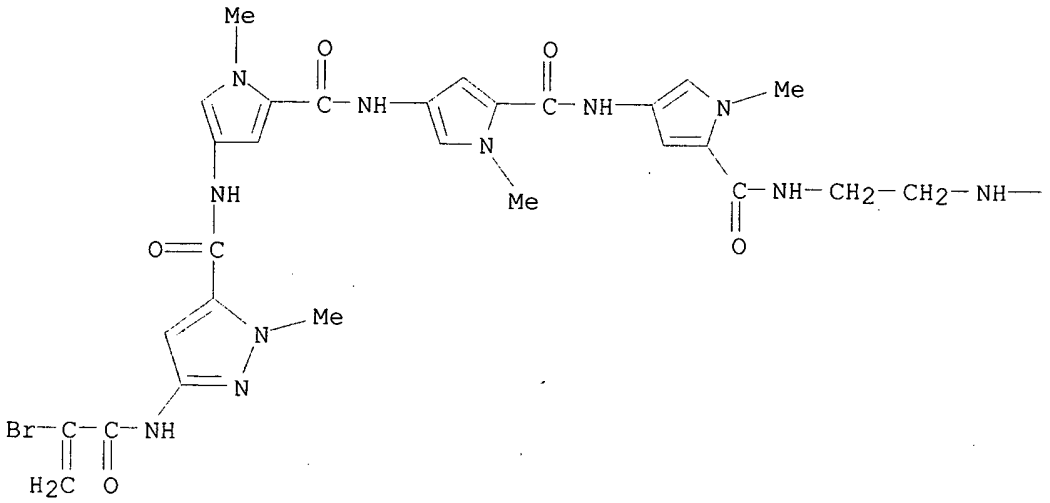


1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

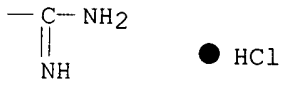
REFERENCE 1: 133:177479

L3 ANSWER 10 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 245046-46-2 REGISTRY
CN 1H-Pyrazole-5-carboxamide, N-[5-[[[5-[[[5-[[[2-[(aminoiminomethyl)amino]ethyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-3-[(2-bromo-1-oxo-2-propenyl)amino]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)
MF C29 H34 Br N13 O5 . Cl H
SR CA
LC STN Files: CA, CAPLUS
CRN (245045-63-0)

PAGE 1-A



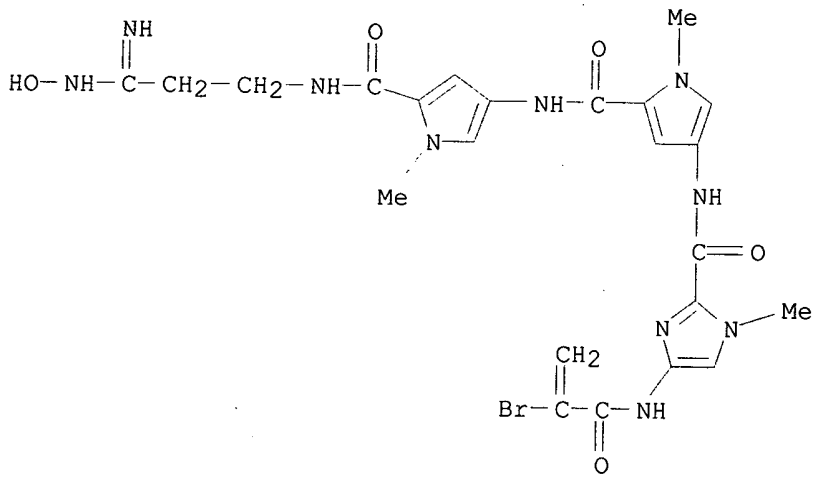
PAGE 1-B



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:257879

L3 ANSWER 15 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 245046-36-0 REGISTRY
CN 1H-Imidazole-2-carboxamide, 4-[(2-bromo-1-oxo-2-propenyl)amino]-N-[5-[[[5-[[[3-(hydroxyamino)-3-iminopropyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-1-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H27 Br N10 O5
SR CA
LC STN Files: CA, CAPLUS

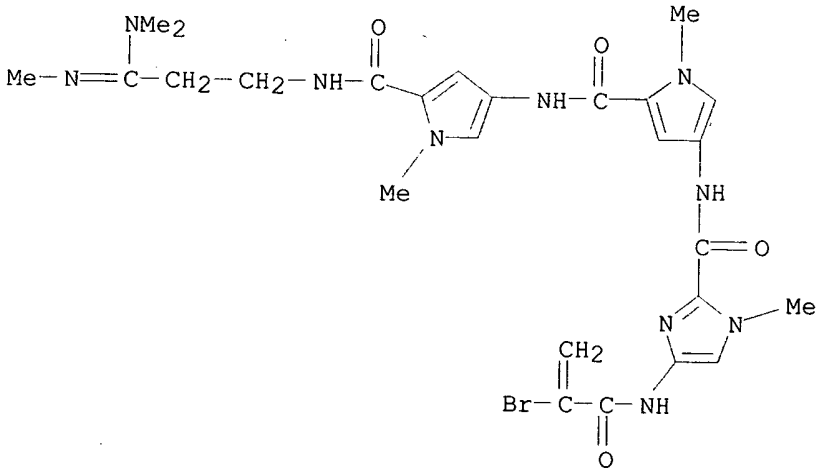


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:257879

L3 ANSWER 20 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 245046-30-4 REGISTRY
CN 1H-Imidazole-2-carboxamide, 4-[(2-bromo-1-oxo-2-propenyl)amino]-N-[5-[[[5-[[[3-(dimethylamino)-3-(methylimino)propyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-1-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C26 H33 Br N10 O4
SR CA
LC STN Files: CA, CAPLUS

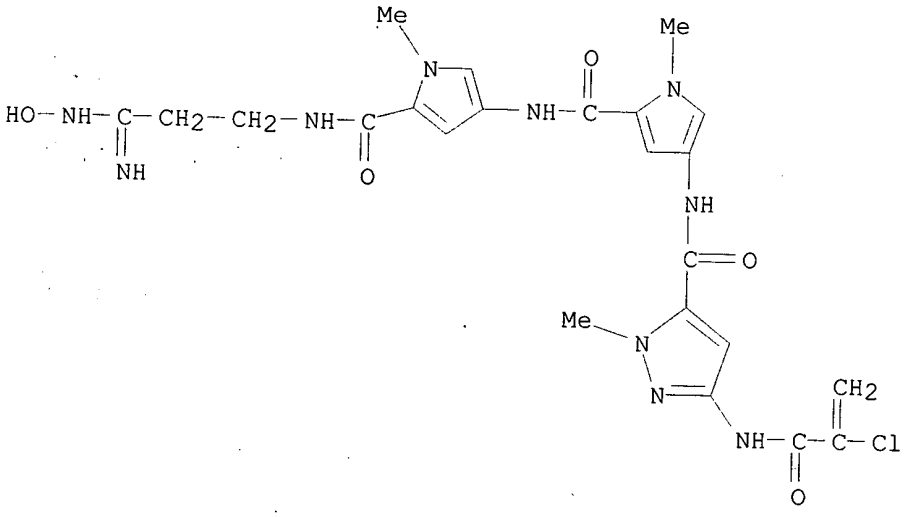


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:257879

L3 ANSWER 25 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 245046-25-7 REGISTRY
CN 1H-Pyrazole-5-carboxamide, 3-[(2-chloro-1-oxo-2-propenyl)amino]-N-[5-[[[5-[[[3-(hydroxyamino)-3-iminopropyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-1-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H27 Cl N10 O5
SR CA
LC STN Files: CA, CAPLUS



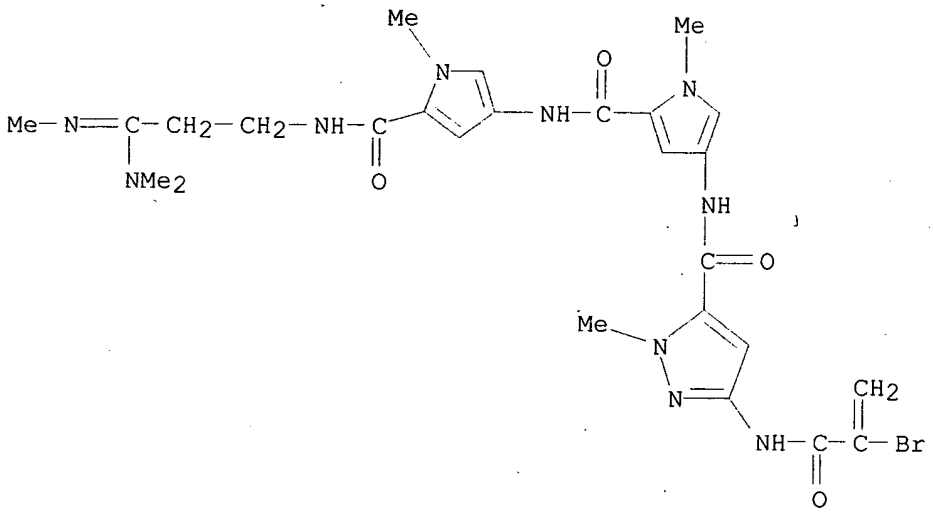
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:257879

L3 ANSWER 30 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 245046-20-2 REGISTRY
CN 1H-Pyrazole-5-carboxamide, 3-[(2-bromo-1-oxo-2-propenyl)amino]-N-[5-[[[5-[[[3-(dimethylamino)-3-(methylimino)propyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-1-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C26 H33 Br N10 O4
SR CA

LC STN Files: CA, CAPLUS



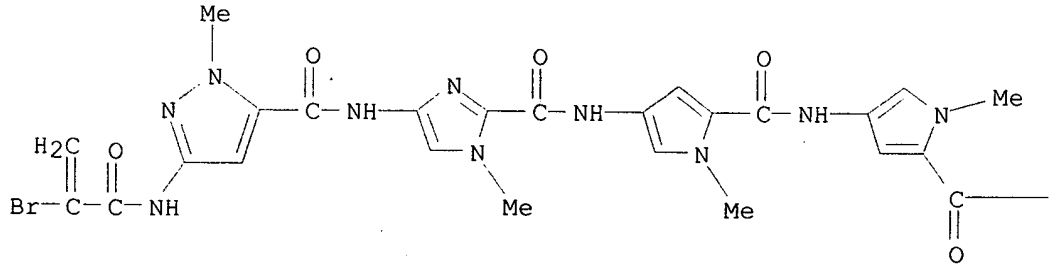
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:257879

L3 ANSWER 35 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 245046-15-5 REGISTRY
CN 1H-Pyrazole-5-carboxamide, 3-[(2-bromo-1-oxo-2-propenyl)amino]-N-[2-[[[5-[[[5-[[(2-cyanoethyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-imidazol-4-yl]-1-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H29 Br N12 O5
SR CA
LC STN Files: CA, CAPLUS

PAGE 1-A



PAGE 1-B

—NH—CH_2—CH_2—CN

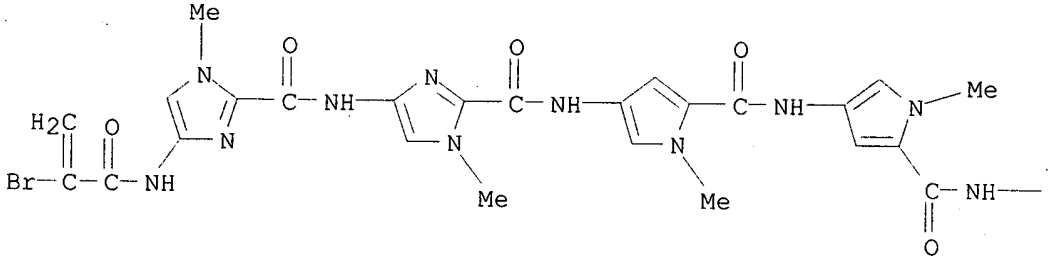
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:257879

L3 ANSWER 40 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 245046-01-9 REGISTRY
CN 1H-Imidazole-2-carboxamide, 4-[(2-bromo-1-oxo-2-propenyl)amino]-N-[2-[[[5-[[[5-[[(2-cyanoethyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-imidazol-4-yl]-1-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H29 Br N12 O5
SR CA
LC STN Files: CA, CAPLUS

PAGE 1-A



PAGE 1-B

—CH_2—CH_2—CN

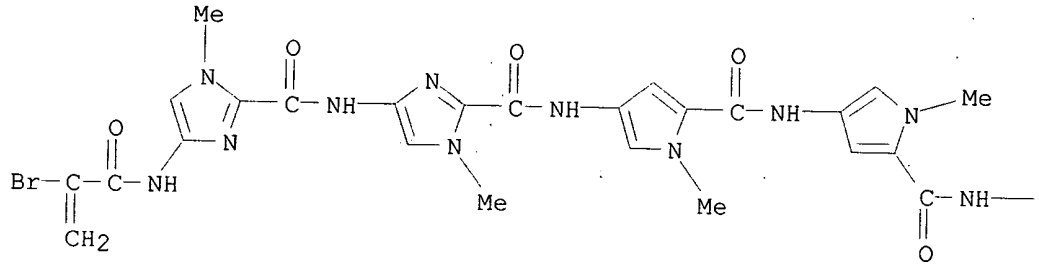
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

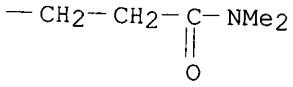
REFERENCE 1: 131:257879

L3 ANSWER 42 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 245045-99-2 REGISTRY
CN 1H-Imidazole-2-carboxamide, 4-[(2-bromo-1-oxo-2-propenyl)amino]-N-[2-[[[5-[[[5-[[[3-(dimethylamino)-3-oxopropyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-imidazol-4-yl]-1-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C30 H35 Br N12 O6
SR CA
LC STN Files: CA, CAPLUS

PAGE 1-A



PAGE 1-B



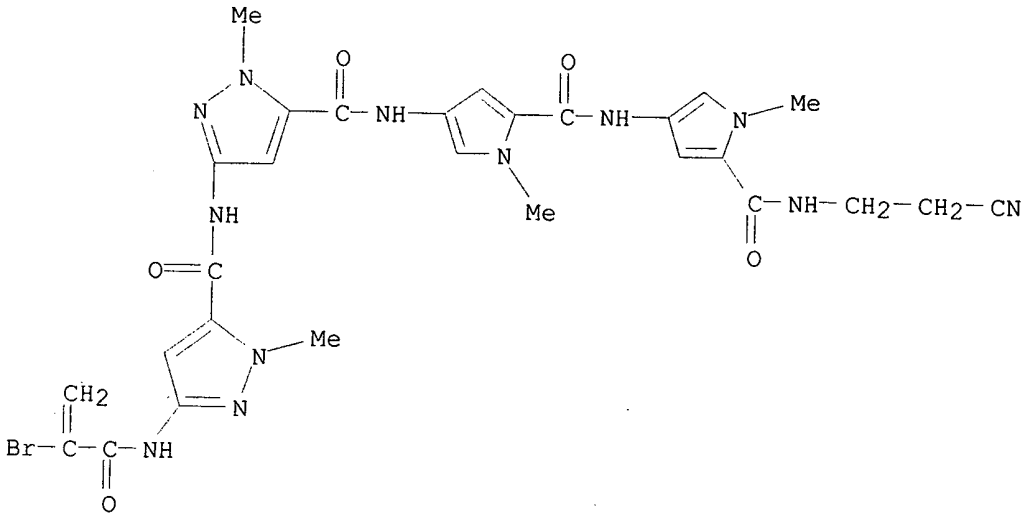
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:257879

L3 ANSWER 45 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 245045-96-9 REGISTRY
CN 1H-Pyrazole-5-carboxamide, 3-[(2-bromo-1-oxo-2-propenyl)amino]-N-[5-[[[5-[[[5-[[(2-cyanoethyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrazol-3-yl]-1-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD

MF C28 H29 Br N12 O5
SR CA
LC STN Files: CA, CAPLUS



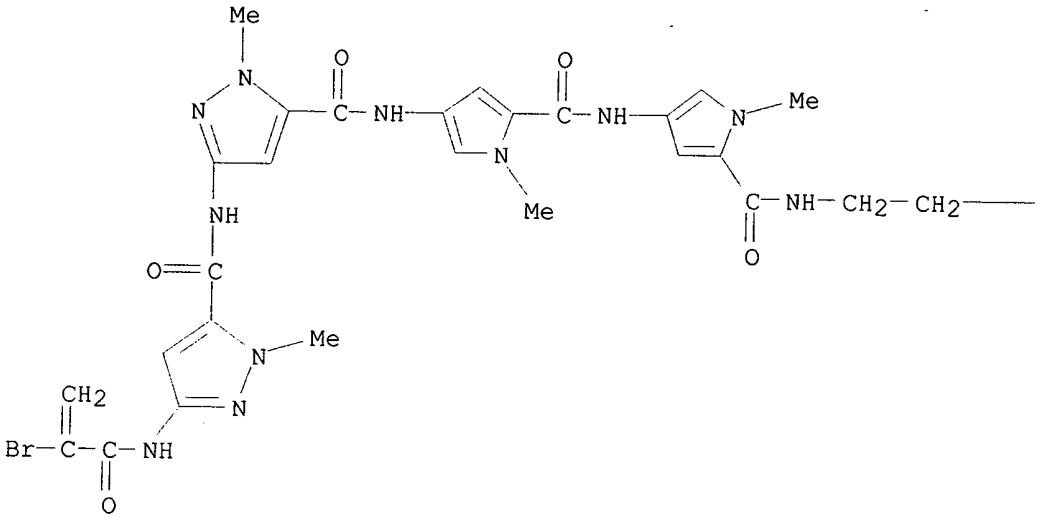
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

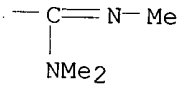
REFERENCE 1: 131:257879

L3 ANSWER 50 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 245045-90-3 REGISTRY
CN 1H-Pyrazole-5-carboxamide, 3-[(2-bromo-1-oxo-2-propenyl)amino]-N-[5-[[[5-[[[5-[[[3-(dimethylamino)-3-(methylimino)propyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrazol-3-yl]-1-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C31 H38 Br N13 O5
SR CA
LC STN Files: CA, CAPLUS

PAGE 1-A



PAGE 1-B



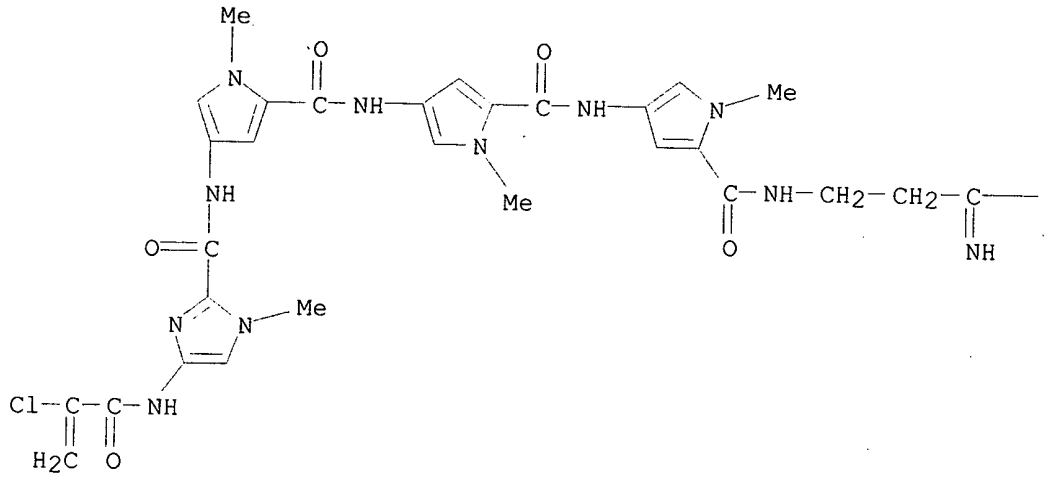
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:257879

L3 ANSWER 55 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 245045-85-6 REGISTRY
CN 1H-Imidazole-2-carboxamide, 4-[(2-chloro-1-oxo-2-propenyl)amino]-N-[5-[[[5-[[[5-[[[3-imino-3-(methoxyamino)propyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-1-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C30 H35 Cl N12 O6
SR CA
LC STN Files: CA, CAPLUS

PAGE 1-A



PAGE 1-B

—NH—OMe

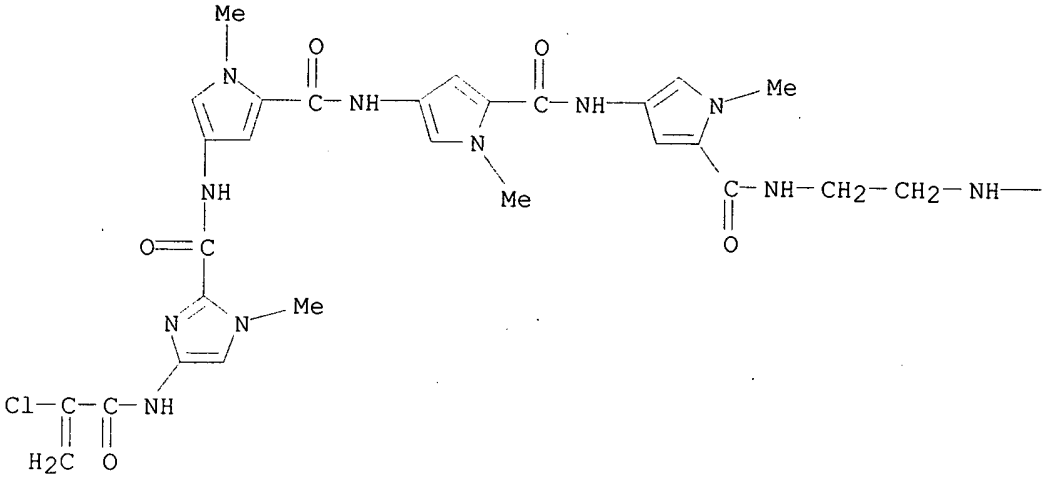
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

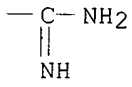
REFERENCE 1: 131:257879

L3 ANSWER 60 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 245045-80-1 REGISTRY
CN 1H-Imidazole-2-carboxamide, N-[5-[[[5-[[[5-[[[2-[(aminoiminomethyl)amino]ethyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-4-[(2-chloro-1-oxo-2-propenyl)amino]-1-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C29 H34 Cl N13 O5
SR CA
LC STN Files: CA, CAPLUS

PAGE 1-A



PAGE 1-B



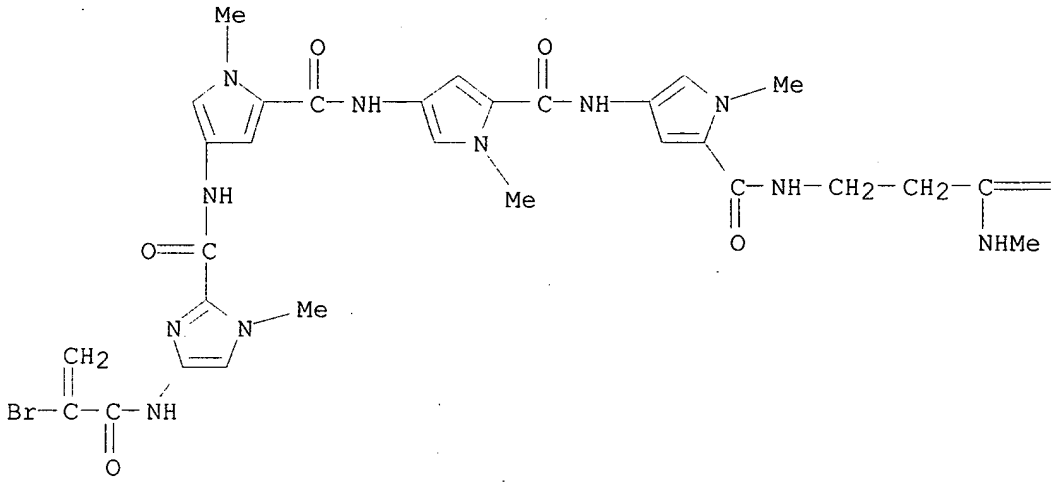
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:257879

L3 ANSWER 65 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 245045-74-3 REGISTRY
CN 1H-Imidazole-2-carboxamide, 4-[(2-bromo-1-oxo-2-propenyl)amino]-1-methyl-N-[1-methyl-5-[[[1-methyl-5-[[[1-methyl-5-[[[3-(methylamino)-3-(methylimino)propyl]amino]carbonyl]-1H-pyrrol-3-yl]amino]carbonyl]-1H-pyrrol-3-yl]amino]carbonyl]-1H-pyrrol-3-yl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C31 H37 Br N12 O5
SR CA
LC STN Files: CA, CAPLUS

PAGE 1-A



PAGE 1-B

=N—Me

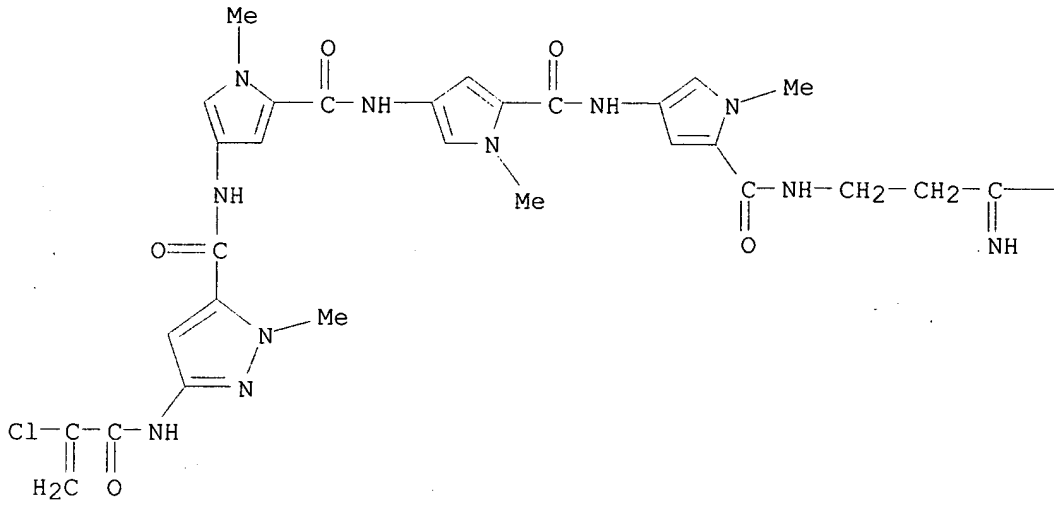
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:257879

L3 ANSWER 70 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 245045-69-6 REGISTRY
CN 1H-Pyrazole-5-carboxamide, 3-[(2-chloro-1-oxo-2-propenyl)amino]-N-[5-[[[5-[[[5-[[[3-imino-3-(methoxyamino)propyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-1-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C30 H35 Cl N12 O6
SR CA
LC STN Files: CA, CAPLUS

PAGE 1-A



PAGE 1-B

— NH— OMe

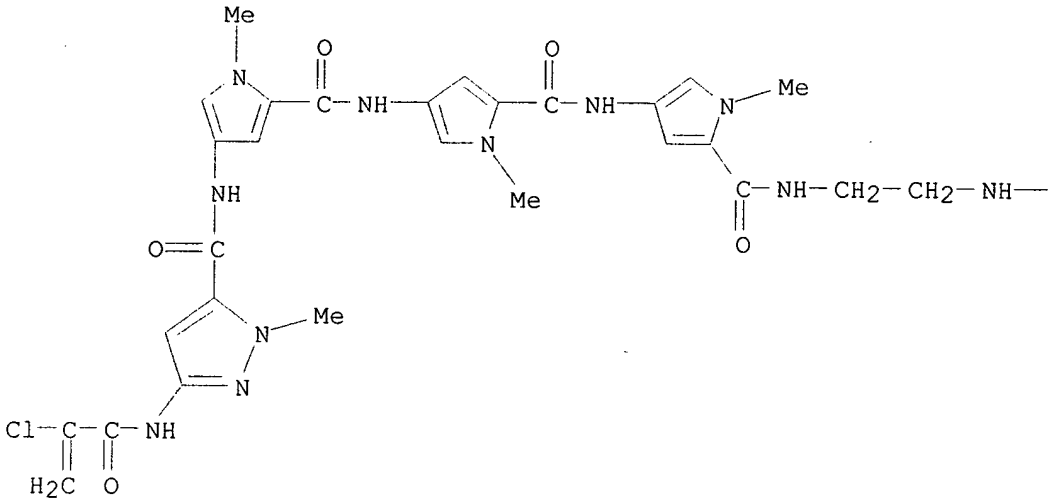
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

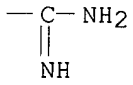
REFERENCE 1: 131:257879

L3 ANSWER 75 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 245045-64-1 REGISTRY
CN 1H-Pyrazole-5-carboxamide, N-[5-[[[5-[[[5-[[[2-[(aminoiminomethyl)amino]ethyl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-3-[(2-chloro-1-oxo-2-propenyl)amino]-1-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C29 H34 Cl N13 O5
SR CA
LC STN Files: CA, CAPLUS

PAGE 1-A



PAGE 1-B



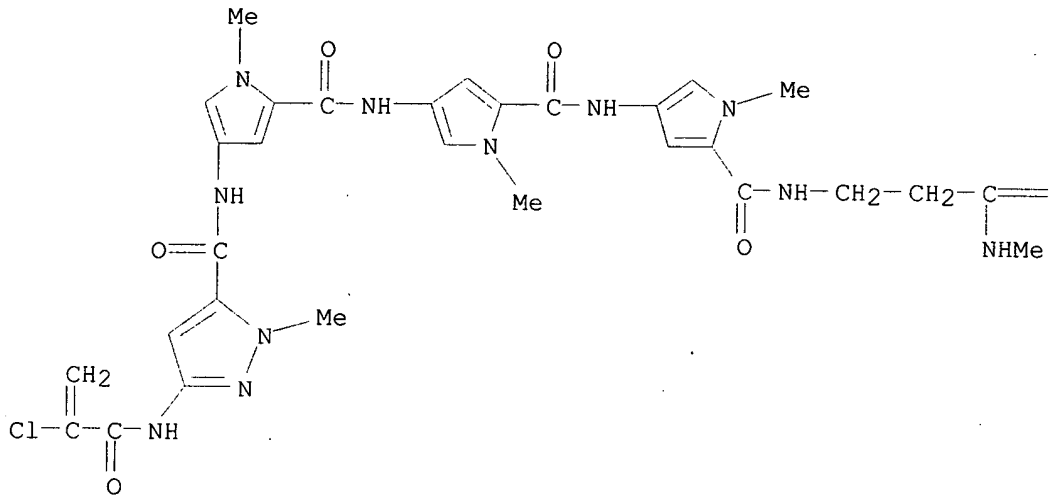
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:257879

L3 ANSWER 80 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 245045-59-4 REGISTRY
CN 1H-Pyrazole-5-carboxamide, 3-[(2-chloro-1-oxo-2-propenyl)amino]-1-methyl-N-[1-methyl-5-[[[1-methyl-5-[[[1-methyl-5-[[[3-(methylamino)-3-(methylimino)propyl]amino]carbonyl]-1H-pyrrol-3-yl]amino]carbonyl]-1H-pyrrol-3-yl]amino]carbonyl]-1H-pyrrol-3-yl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C31 H37 Cl N12 O5
SR CA
LC STN Files: CA, CAPLUS

PAGE 1-A



PAGE 1-B

=N—Me

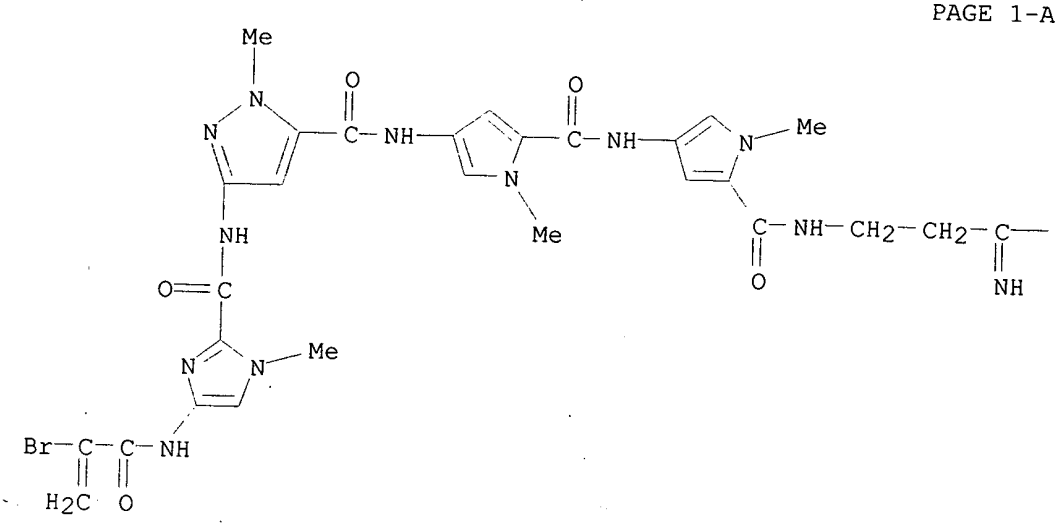
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 131:257879

L3 ANSWER 85 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 177410-01-4 REGISTRY
CN 1H-Pyrazole-5-carboxamide, N-[5-[[[5-[[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-3-[[[4-[(2-bromo-1-oxo-2-propenyl)amino]-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H32 Br N13 O5
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

PAGE 1-A



PAGE 1-B

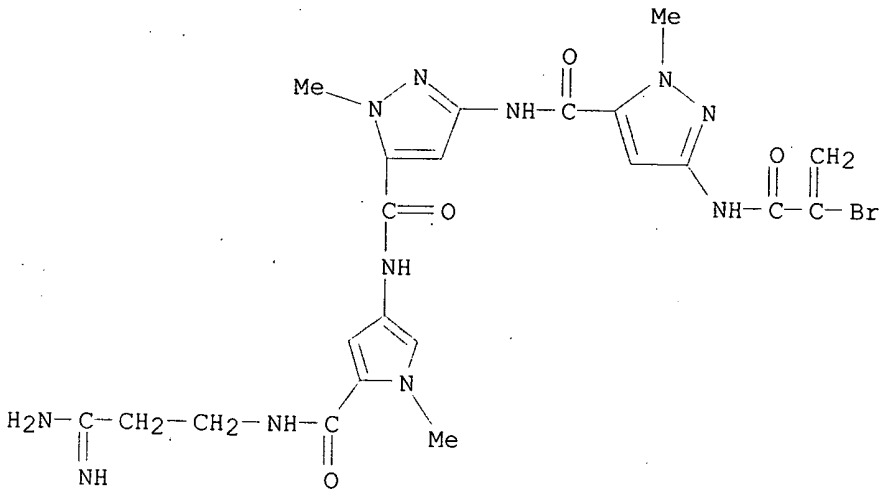
—NH_2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:10484

L3 ANSWER 86 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 177409-99-3 REGISTRY
CN 1H-Pyrazole-5-carboxamide, N-[5-[[[5-[[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrazol-3-yl]-3-[(2-bromo-1-oxo-2-propenyl)amino]-1-methyl-(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C22 H26 Br N11 O4
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

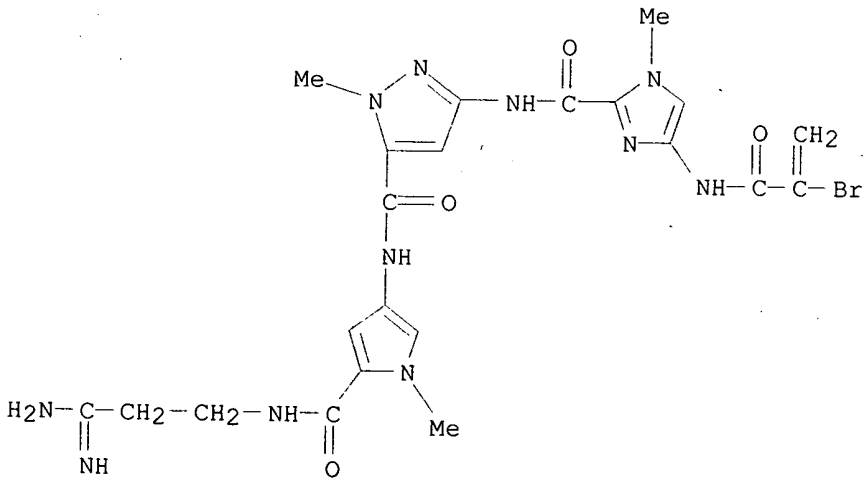


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:10484

L3 ANSWER 90 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 177409-84-6 REGISTRY
CN 1H-Pyrazole-5-carboxamide, N-[5-[[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-3-[[[4-[(2-bromo-1-oxo-2-propenyl)amino]-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C22 H26 Br N11 O4
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



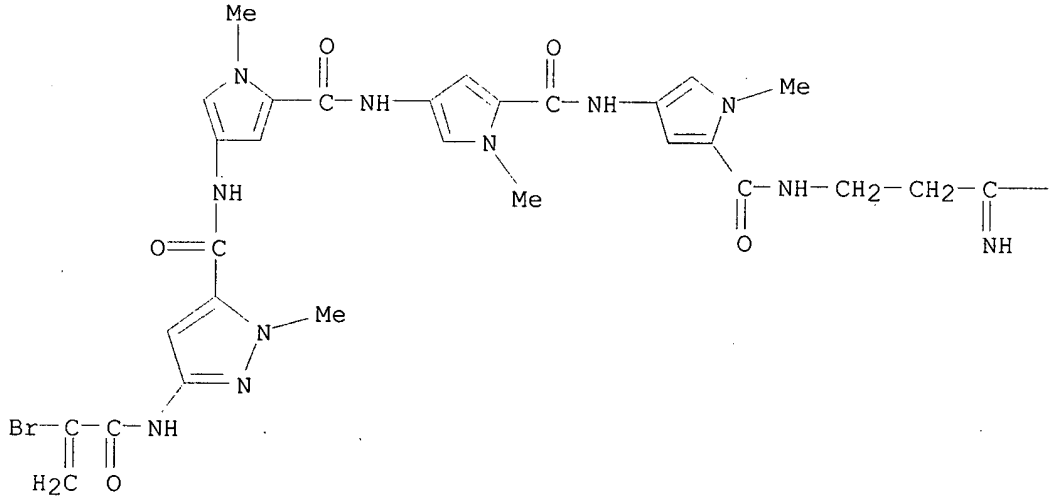
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:10484

L3 ANSWER 95 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 177409-55-1 REGISTRY
CN 1H-Pyrazole-5-carboxamide, N-[5-[[[5-[[[5-[[(3-amino-3-iminopropyl)amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]amino]carbonyl]-1-methyl-1H-pyrrol-3-yl]-3-[(2-bromo-1-oxo-2-propenyl)amino]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)
MF C29 H33 Br N12 O5 . Cl H
SR CA
LC STN Files: CA, CAPLUS, TOXLIT, USPATFULL
CRN (177409-88-0)

PAGE 1-A



PAGE 1-B

— NH_2

HCl

4 REFERENCES IN FILE CA (1967 TO DATE)
4 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:232356

REFERENCE 2: 131:257879

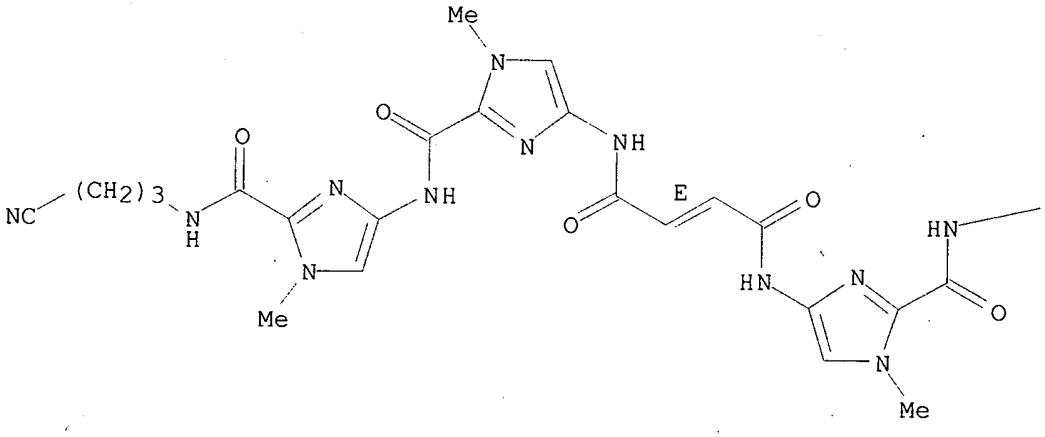
REFERENCE 3: 125:143280

REFERENCE 4: 125:10484

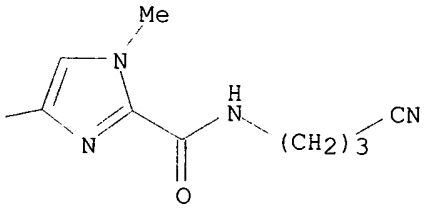
L3 ANSWER 97 OF 97 REGISTRY COPYRIGHT 2001 ACS
RN 142482-49-3 REGISTRY
CN 2-Butenediamide, N,N'-bis[2-[[[2-[[(3-cyanopropyl)amino]carbonyl]-1-methyl-1H-imidazol-4-yl]amino]carbonyl]-1-methyl-1H-imidazol-4-yl]-, (E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C32 H36 N16 O6
SR CA
LC STN Files: CA, CAPLUS

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 117:112029